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Flow through a laboratory sediment sample by computer simulation modeling

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Abstract

A laboratory sediment sample is digitized by X-ray computed tomography system to obtain a host matrix of size 100^3 of porosity 0.282. Flow through the porous medium is studied by an interacting lattice gas model for fluid driven by pressure bias. The bias $H(0 \leqslant H \leqslant 1)$ is implemented via soft and hard pressure constraints in selecting the stochastic movement of fluid particles. The response of fluid flux density to bias H is nearly linear with soft pressure; it becomes nonmonotonic with the hard pressure.
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Keywords: Porous medium formed by quartz sands; Interacting lattice gas; Computer simulation; Driven flow

Understanding the flow through porous media has attracted a considerable interest [1–4] for decades due to its complex response properties. Some applications include secondary oil recovery, spreading of spilled contaminants, and dissociation of gas (methane, carbon monoxide, etc.) in natural occurring processes [5]. Heterogeneous porous media for geomarine applications are generally modeled by percolation [6] and its variants. Transport and flow through such porous matrices have been extensively studied near and above the percolation threshold [7,8]. Scaling behavior of such response properties as the variation of the flux density with porosity, driving bias, temperature, etc. are relatively well understood. However, fluid flow through a laboratory sample [9,10] may differ from that in an idealized percolating porous matrix. Our goal is to understand realistic porous media and characterize its flow properties such as transport of fluid and hydraulic conductivity. The porous matrix is prepared in the laboratory from distribution of quartz sands with appropriate geomarine environmental conditions such as pressure, compaction, and temperature. Enormous efforts have been made in recent years to study structural patterns and flow of such granular materials in a variety of driving mechanisms such as vibrations, mixing, shearing, etc. by both computer simulations and

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14. ABSTRACT

Understanding the flow through porous media has attracted a considerable interest [1–4] for decades due to its complex response properties. Some applications include secondary oil recovery, spreading of spilled contaminants, and dissociation of gas (methane, carbon monoxide, etc.) in natural occurring processes [5]. Heterogeneous porous media for geomarine applications are generally modeled by percolation [6] and its variants. Transport and flow through such porous matrices have been extensively studied near and above the percolation threshold [7,8]. Scaling behavior of such response properties as the variation of the flux density with porosity, driving bias, temperature, etc. are relatively well understood. However, fluid flow through a laboratory sample [9,10] may differ from that in an idealized percolating porous matrix. Our goal is to

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laboratory experiments [11–16]. We are focused on characterizing the flow through the network of pores formed from the granular sands, i.e., the laboratory sample, using a computer simulation model. Relatively few attempts [9] are made to carry out such studies of flow through such a laboratory porous medium. The distributions of sediments (barriers) and network of pores (pathways) in our laboratory sample are identified by X-ray computed tomography measurements. Using a digitized image of the sample as a host matrix, attempts are made to characterize its flow properties and hydraulic conductivity via an interacting lattice gas method.

We consider a cubic lattice of size L^3 with $L = 100$, the digitized laboratory sample with a source of fluid particles connected to the bottom of the lattice ($z = 1$). The sediment sites act as impenetrable immobile barriers while the nearest-neighbor pore sites attract the mobile hard-core fluid particles. The interaction energy between a particle and its adjacent pore site is taken to be $J = -1$. The molecular weight of fluid constituents ($M = 0.1$, relatively small here) facilitates the downward ($-z$) fall and resist the upward ($+z$) move via change in the gravitational potential energy ($M\Delta z, \Delta z = \pm 1$). The change in energy (interaction and gravitational) is used in the Boltzmann distribution at a fixed temperature ($T = 1$) in implementing the move by the Metropolis algorithm. The source of fluid particles at the bottom creates a high concentration gradient which drives the particles upward against gravity. Additionally, we consider hydrostatic pressure bias (H) to drive these constituents upward (follows).

Selection of an adjacent neighboring site along the transverse ($\pm x, \pm y$) and vertical ($\pm z$) directions for a particle's move depends on the bias. Three types of bias are considered with $0 \leqslant H \leqslant 1$ which could be used to describe different senario as explained briefly below.

I: Hopping probability along the transverse directions remains independent of bias which controls only the longitudinal moves. The bias along the longitudinal direction decreases with the height (z) with a linear gradient.

$$P_x = P_{-x} = P_y = P_{-y} = \frac{1}{6}, \quad P_{-z} = \frac{1 - H[1 - (z/L)]}{6}, \quad P_z = \frac{1 + H[1 - (z/L)]}{6}. \tag{1}$$

The bias is linear with the height z with the largest at $z = 0$. Even at the largest value of bias, $H = 1$, the maximum hopping probability along z-direction cannot exceed $\frac{1}{3}$. Since the selection of nearest-neighbor site for hopping along the transverse directions ($\pm x, \pm y$) remain independent of bias, it is not feasible to implement extreme bias that can channel fluid flow only along one direction.

II: The hopping along the longitudinal direction depends on the bias but becomes independent of the height while maintaining the constant hopping rate along the transverse directions.

$$P_x = P_{-x} = P_y = P_{-y} = \frac{1}{6}, \quad P_{-z} = \frac{1 - H}{6}, \quad P_z = \frac{1 + H}{6}. \tag{2}$$

III: Hopping along all directions are coupled with bias such that at extreme value of the bias ($H \to 1$), probability of selecting a hopping site along the positive longitudinal direction approaches one and zero along the rest.

$$P_x = P_{-x} = P_y = P_{-y} = P_{-z} = \frac{1 - H}{6}, \quad P_z = \frac{1 + 5H}{6}. \tag{3}$$

With this bias, one can examine a much larger range in channeling the flow. Thus, with these three bias one should be able to study flow in a large pool of systems.

To implement the hopping [7,8], we select a particle say at a lattice site i randomly. One of its six nearest-neighbor sites say j is selected with above probability. If site j is empty then an attempt is made to move the particle from site i to site j with the Metropolis algorithm. Periodic boundary conditions are used along the transverse direction; both the top ($z = L$) and the bottom ($z = 1$) of the sample are open for particles to escape. A particle is released from the source into a bottom lattice site as soon as it is vacated by the particle when it moves up or diffuses laterally. As usual, attempts to move each particle once define the unit Monte Carlo step (MCS) time. As the simulation proceeds, particles move in and out of the sample. The number of particles and their concentration profiles (planar densities along x, y, z) change but eventually reach a steady-state—a non-equilibrium steady-state system. Simulations are performed with many independent initial configurations but with the same host matrix, each for a sufficiently long time steps to reach steady-state.
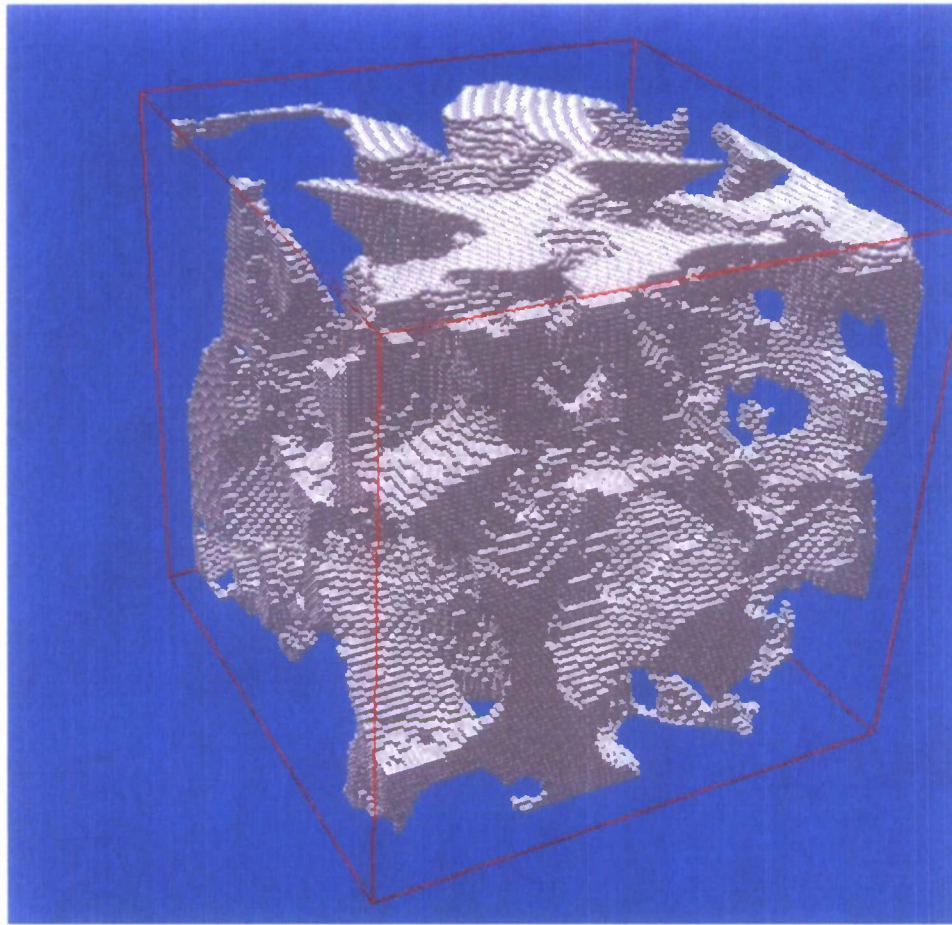
Fig. 1. Distribution of pores in the sample 100^3 from quartz sand grains (see **Fig. 2** for details).

The laboratory sample is relatively dense with a fraction of sediment barriers $p_b = 0.718$ and pore sites $p_o = 0.282$. Thus, it would be better to look at the porous medium with empty sites of the sample. **Fig.** 1 shows the distribution of pores in the digital sample. Note that the fraction of pore sites is below the site percolation threshold ($p_c \simeq 0.3117$) [6], yet we have connected pathway of pores that span the entire sample. Obviously, open channels in the real sample are different from the idealized percolating matrix with random distribution of barriers in a site percolation. To depict the contrast and complementarity in distribution of sediments and pores, in **Fig.** 2 we present a slice of the sample with distribution of its sediment and pore sites.

We perform the computer simulation experiment by injecting fluid at one end and monitoring its net flux rate from the opposite end by varying the bias for three types of driving mechanisms described above. During the simulation, we also keep track of the root mean square (rms) displacement of each particle (tracer) and their center of mass, density profiles, and flux of fluid. **Fig.** 3 shows the variation of the rms displacement with the time steps (t) for a range of bias values with pressure bias III. We see that particles, individually (tracer) and collectively (center of mass) drift, i.e., $R \propto t$, in the long time (asymptotic) regime. Such an asymptotic drift behavior is expected in the long time regime for our driven system due to pressure bias and concentration gradient. Note that the asymptotic drift behavior also suggests that the system has reached its steady-state which is verified by the analysis of flux density in the following.

There is a net mass transfer due to net driving field (along $+z$ direction) caused by (1) the concentration gradient developed by the source at the bottom and (2) the pressure bias. Fluid particles enter at the bottom and leave mostly from the top. The amount of fluid entering the system must be equal to amount leaving in the steady-state due to conservation of mass, i.e., the continuity equation. The fluid current i can be estimated
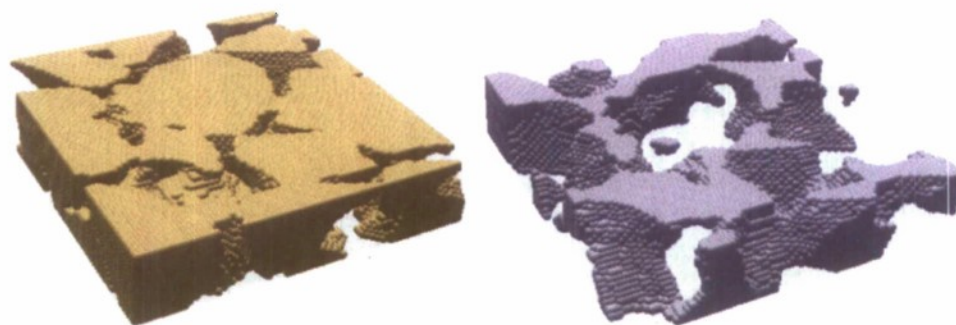
Fig. 2. Distribution of sediment (left) and pores (right) in slices of equal thickness at $z = 21–40$ in the sample which is prepared from quartz sand grains. The sandy sediments are collected from surficial marine deposits. Sediments are subrounded to subangular in shape have a mean grain size or d_{50} of 0.375 mm and serve as the boundaries for the pores (right).
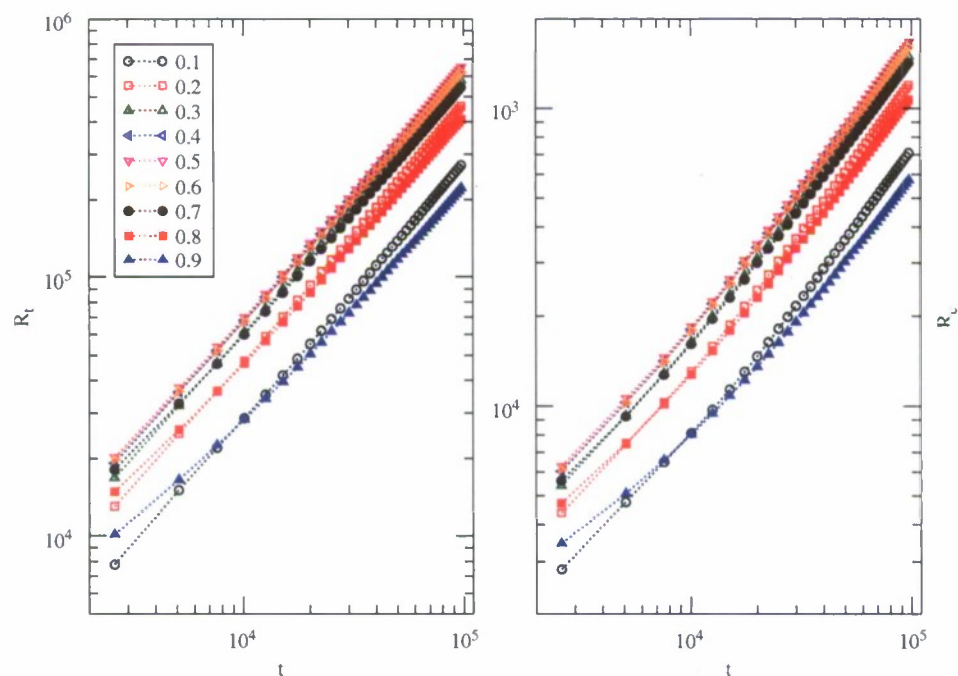

Fig. 3. Variation of the root mean square displacement of each particle (tracer), R_t and their center of mass (right), R_c with bias III on sample shown in **Fig.** 1.

from the rate of net mass (Q) transfer,

$$i = \frac{\mathrm{d}Q}{\mathrm{d}t}. \tag{4}$$

The current or flux density (j) is the current per unit cross-sectional area (A_C),

$$j = i/A_C. \tag{5}$$

The flux density is linearly proportional to hydraulic conductivity (κ) for flow with linear response (with $\delta = 1$),

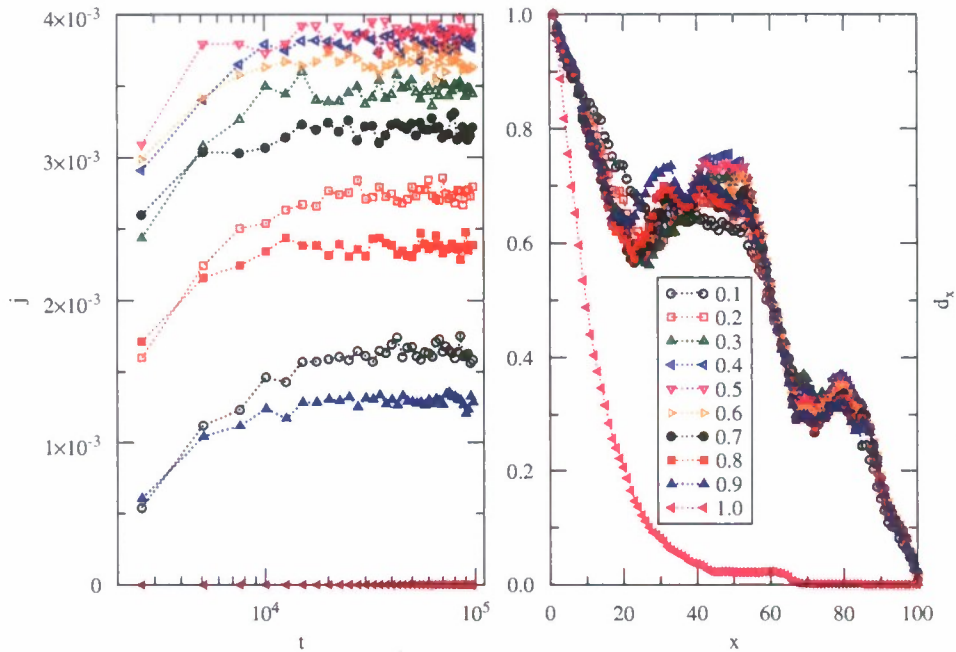$$j = \kappa H^{\delta}. \tag{6}$$

Fig. 4. Variation of the mass flux density rate (left) and longitudinal (along bias) density profile with bias III.
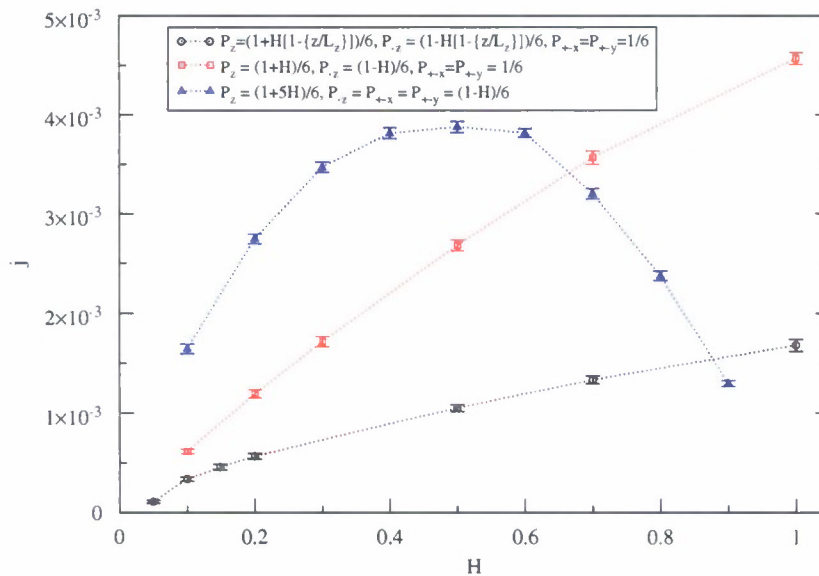

Fig. 5. Variation of the steady-state value of flux density with bias H for three types I, II, III.

Variation of the flux density with the time step is presented in **Fig. 4** for the entire range of a bias (III). We see that the flux density reaches its constant value rather fast. Corresponding density profiles are also shown in this figure. The non-linear density profiles are mostly due to morphology of the pore distribution except at extreme bias $H = 1$. Movement of fluid particles ceases as they are trapped against sediment barrier at the extreme value of type III bias.

Response of the flux density to the bias can be analyzed by examining the variation of its steady-state value with the bias. **Fig. 5** shows the variation for three types of pressure bias. For bias I and II, we see relatively

linear responses of the flux density to bias while for bias III, a non-monotonic dependence is observed. Note that in case of bias I and II, the hopping probability of fluid constituents along the transverse directions never ceases even at extreme values of the bias. With the pressure bias III, the movement in all directions except z ceases at $H = 1$. We believe that the implementation of the pressure bias III is more realistic in directing the flow which shows a non-monotonic response of the flux density. We are in a process to carry out both laboratory and computer simulation experiments simultaneously to see which bias is more appropriate in describing the flow properties of the porous sediment.

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